# Novel Ionic Liquids for $CO_2$ Capture: Computational Design to Laboratory Demonstration

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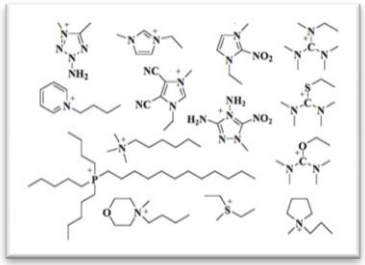
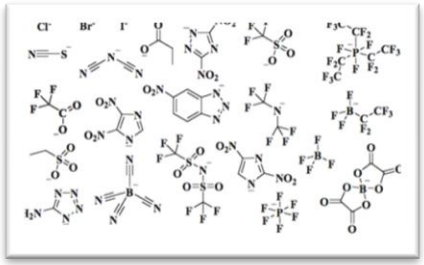
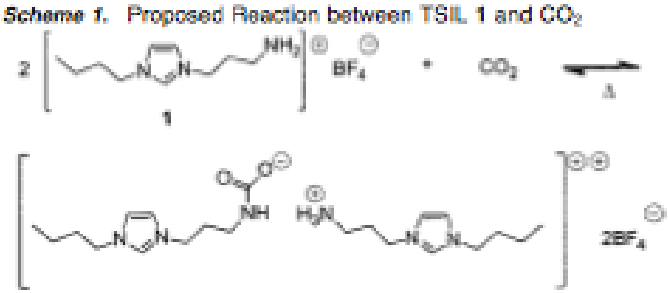
- Non-aqueous solvents desirable for $CO_2$ separations
- Ionic liquids are ambient temperature liquid organic salts
  - Bulky organic cations and anions
  - Unlimited diversity of potential compounds
- Why investigate ionic liquids for $CO_2$ capture?
  - IL physical properties favorable for $CO_2$ capture
  - Negligible volatility
  - High intrinsic physical selectivity for $CO_2$
- $CO_2$-specific chemical functionality readily introduced
  - "Task-specific ionic liquids" (TSILs)



*Common IL cations*



*Common IL anions*

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**$CO_2$ Capture by a Task-Specific Ionic Liquid**

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**Problems with existing $CO_2$ TSILs**

- Lack of reaction energy "tunability"
- Potentially complex reaction stoichiometry
- Very high viscosity in reacted state

**Key project elements**

- Computationally design new TSILs that have properties tuned for CO2 capture
  - Electronic structure, classical atomistic simulations
- Apply state-of-the-art experimental tools to determine ionic liquid physical properties
  - Synthesis, property measurement, characterization
- Tightly integrate process modeling with molecule discovery efforts
  - HYSYS, Aspen